

1. **Research Title:** Machine Learning for Polymer Solution Processing and Design

2. **Individual Sponsor:**

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3. **Academic Area/Field and Education Level**

Chemical Engineering, Material Science, Physics, Computer Science,  
Machine Learning, or related field.

4. **Objectives:** Develop and test data-centric and/or physics-integrated machine learning models for predicting polymer solution properties

5. **Description:** Polymers are widely used in various technological applications for air and space applications including high-temperature polyimides, polyelectrolytes, and sequence-based or complex-shaped polymers. These materials are often processed, synthesized, or designed in solution, where the resulting material performance and characterization depends on solvent quality, experimental conditions (e.g. temperature, pressure, etc.), polymer chemistry and kinetics, among other factors. Much of our understanding on how these processes affect the macroscopic design is limited, and the ability to predict polymer solution properties such as their dynamics, self-assembly, and phase behavior is crucial to the control over morphology and structure. Machine learning models are becoming more widely used in predicting polymer properties but require sufficient quality data. This research aims to integrate physics-based machine learning models to elucidate the effect of polymer chemistry, state variables, and other thermodynamic properties on their dynamics in solution. Key interests include the self-assembled structure, morphology, phase behavior, and dynamics of polymers during solution processing and to develop interpretable machine learning models for predicting new physics in unseen polymer systems. Techniques include regression and classification machine learning, molecular dynamics simulations, and high-throughput experimentation/modeling methods for accelerating data availability.

6. **Research Classification/Restrictions:** Unclassified and unrestricted

7. **Eligible Research Institutions:** Any

8. **PA Approval #:** AFRL-2023-4198